Topological Analysis Of The Electron Density Through The Bader Theory

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Syllabus:

- Basic concepts of the Bader theory
- Implementation of the topological analysis
- Bader analysis in solid systems:
  - Charge
  - LDOS
- Conclusion and Acknowledgements

Bader Theory
Basic Concepts

Define the charge of the atom-in-the molecule <u>without ambiguity</u>

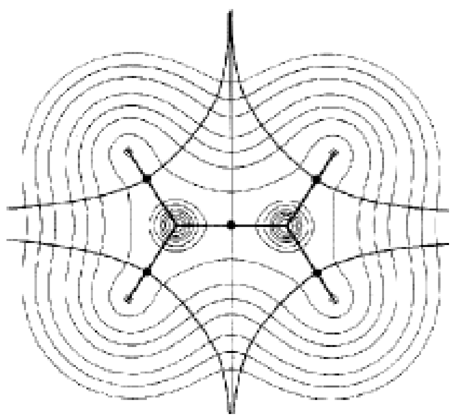
Example : C_2H_4

http://www.chemistry.mcmaster.ca/faculty/bader

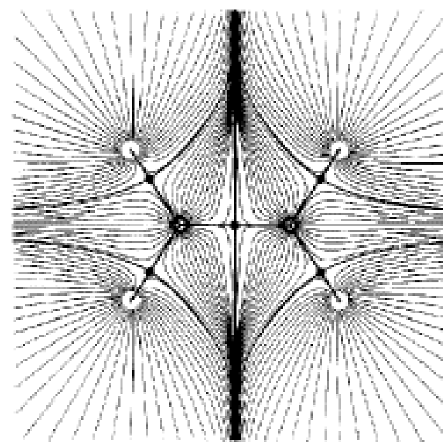
Inter-atomic surfaces:
zero flux condition

$$\nabla \rho(r) \bullet n(r) = 0$$

ρ(r)



• ρ(r)



Bond-critical points :

$$\nabla^2 \rho\,(r_{BCP}) > 0 \;\; // \text{ bond}$$

$$\nabla^2 \rho\,(r_{BCP}) < 0 \;\; \perp \text{ bond}$$

- Integration of ρ(r) inside atomic basins yields charge Q
- Integration of wave functions yields LDOS

Bonds are defined on the basis of the electron distribution : no arbitrary cut-off

Inspection of $\rho\,(r_{BCP})$ gives information on the ionic/covalent nature of the bond

The Implementation of The Bader theory

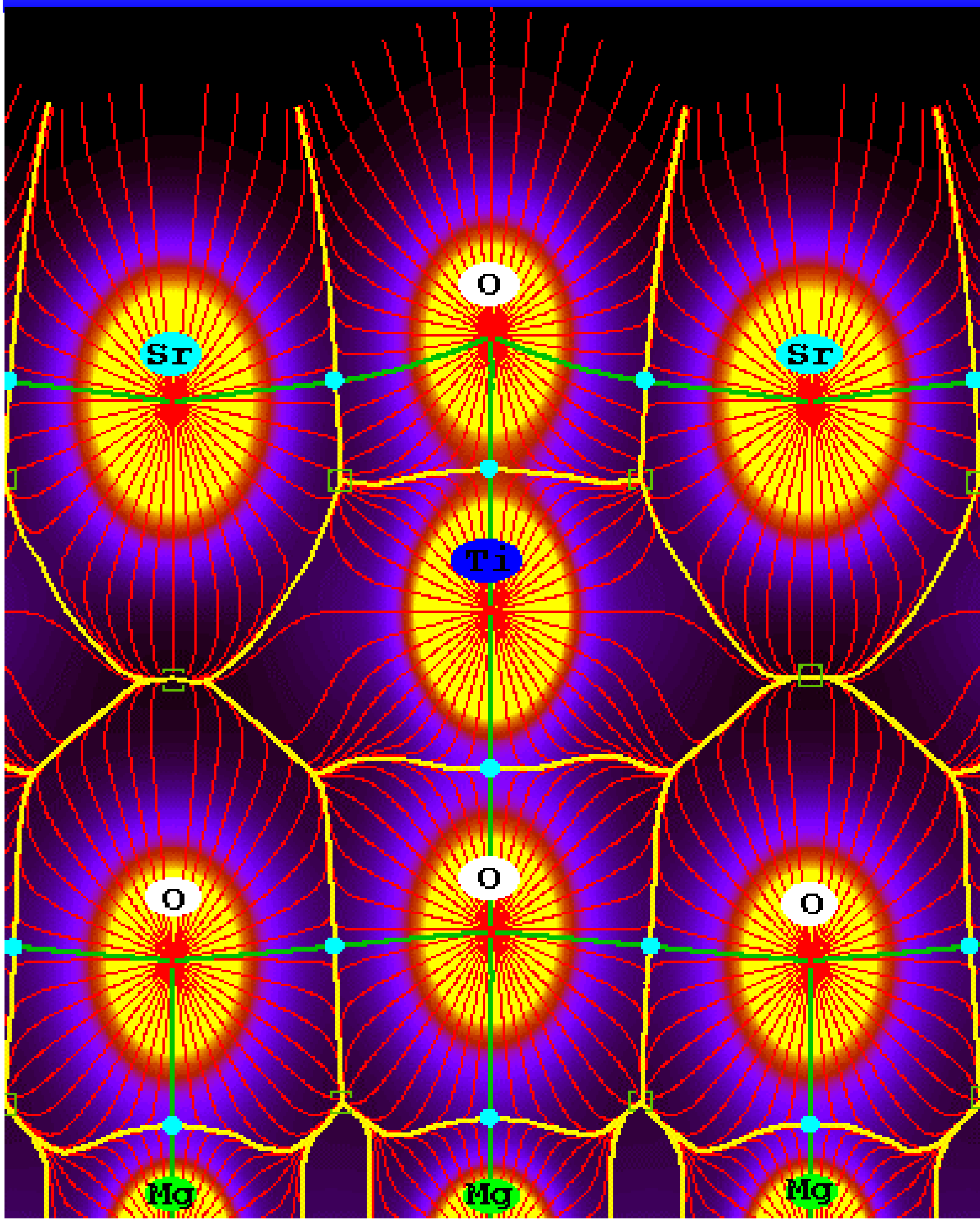
- Input
  - ABINIT => valence density output file
  - FHI98PP => core density files
- Implementation
  - 3D real space interpolation scheme based on the cubic splines in 1D
  - Independent handling of the core and valence density
- Algorithm (to be repeated for each atom)
  - CP searching - Popellier algorithm :

    nucleus => (3,-1) =>(3,1)=>(3,3)
  - Determination of the Bader radius as a function of the polar and azimuthal angles (starting near the CP) – the procedure taking most of the time!
  - Integration of the charge (or other quantities) inside the Bader surface

Note: there may be atom-like attractors even in absence of nuclei (ex: O vacancies in oxides).

Bader Analysis

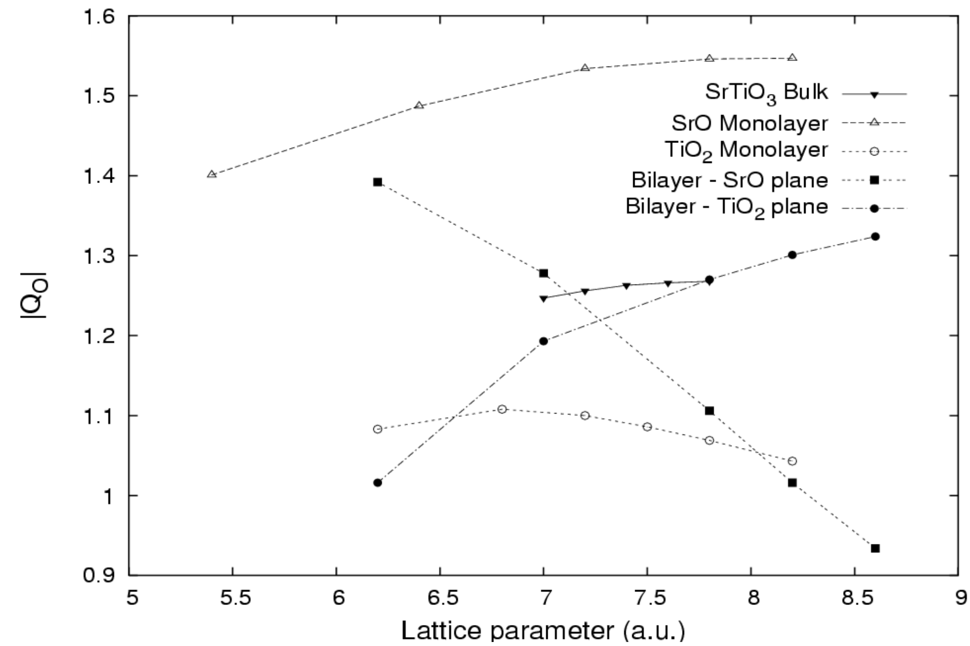
Sr0-TiO$_2$-MgO(001) – (110) plane



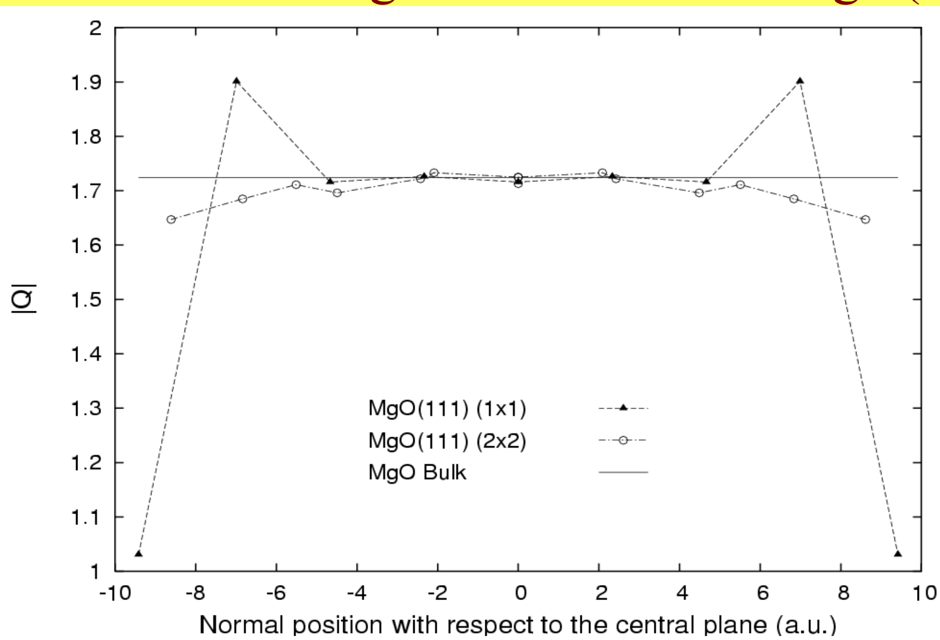
Bader Charge

some examples

Charge of Oxygen in different environments

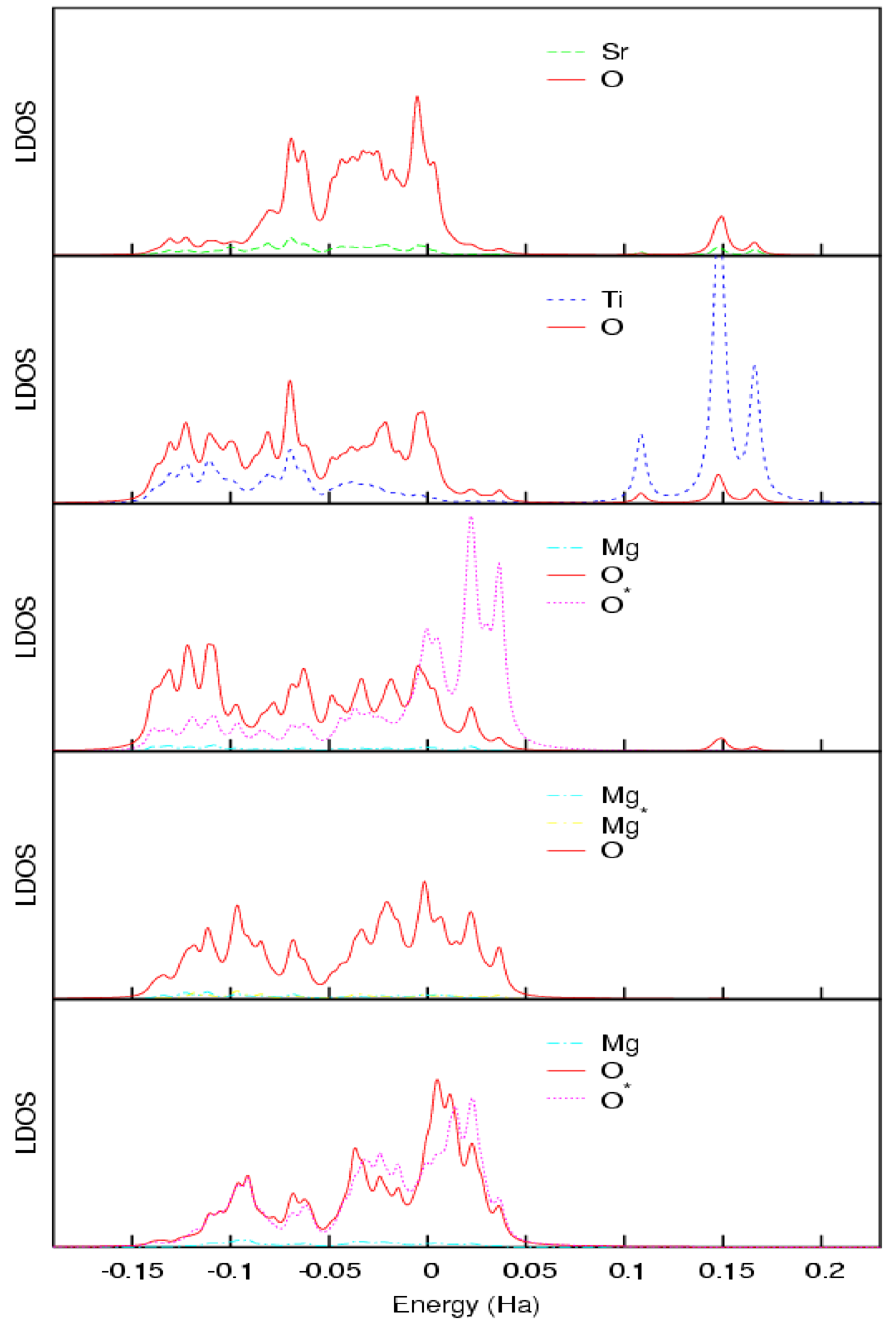


Variation of the charge at the surface - MgO(111)



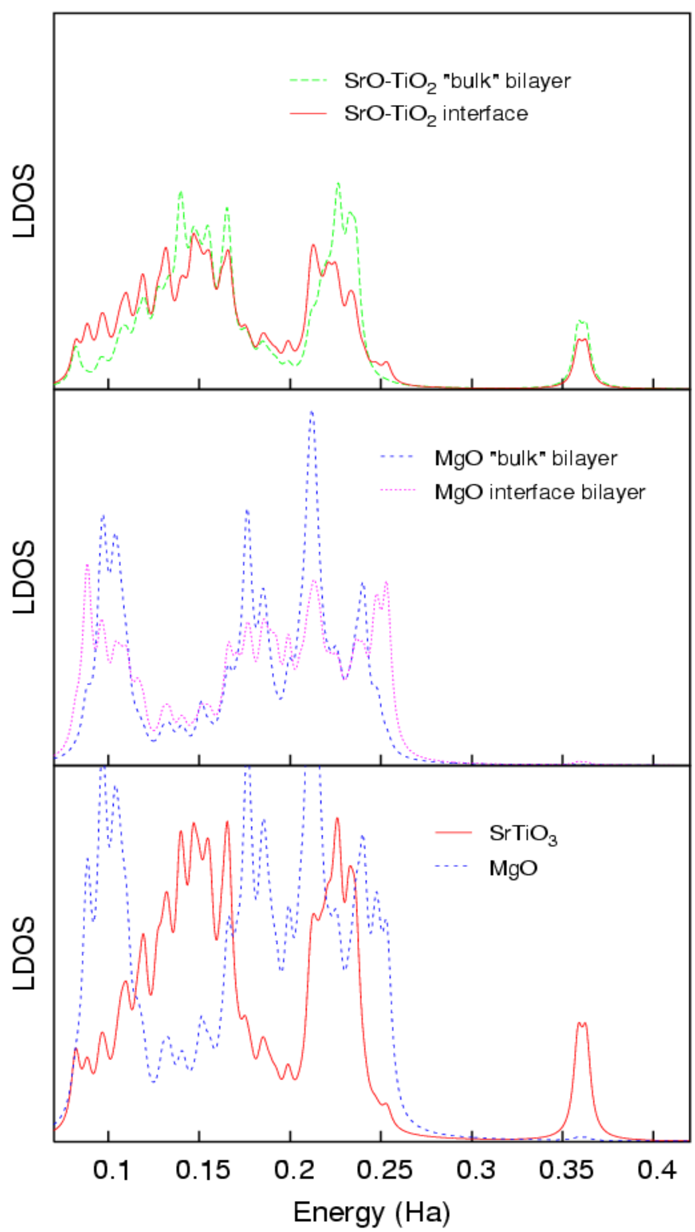
LDOS Of The Bader Atom

SrO-TiO_2-MgO(3) -LDOS analysis



Band-offset Analysis
(preliminary results)

$SrTiO_3$-MgO(001) Interface (7+7 superlattice)



Conclusion

Implemented in ABINIT:

- Critical point analysis
- Determination of the Bader surface
- Calculation of the Bader charges and the volume of the atomic basins

Developments

- LDOS analysis
- Visualisation

Acknowledgments

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- Xavier Gonze for help with the implementation to ABINIT
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